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Demonstrating fractal scaling of residence time distributions on the catchment scale using a fully-coupled, variably-saturated groundwater and land surface model and a Lagrangian particle tracking approach

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ABSTRACT - The influence of the vadose zone, land surface processes, and macrodispersion on scaling behavior of residence time distributions (RTDs) is studied using a fully coupled watershed model in conjunction with a Lagrangian, particle-tracking approach. Numerical experiments are used to simulate groundwater flow paths from recharge locations along the hillslope to the streambed. These experiments are designed to isolate the influences of topography, vadose zone/land surface processes, and macrodispersion on subsurface RTDs of tagged parcels of water. The results of these simulations agree with previous observations that RTDs exhibit fractal behavior, which can be identified from the power spectra. For cases incorporating residence times that are influenced by vadose zone/land surface processes, increasing macrodispersion increases the slope of the power spectra. In general the opposite effect is demonstrated if the vadose zone/land surface processes are neglected. The concept of the spectral slope being a measure of stationarity is raised and discussed.

Introduction

The observation by Kirchner et al. [2000] that long-term time series of stream chemistry exhibit fractal behavior has prompted increased interest in residence time distributions of groundwater from the streambed scale (10^0m) to the continental scale (10^6m) [e.g., *Worman et al.*, 2007]. The main focus of previous work has been on the role of

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subsurface heterogeneity in solute transport [*Haggerty et al.*, 2000; *LaBolle et al.*, 2006; *Maxwell et al.*, 2003; *Tompson et al.*, 1999], the patterns of vegetation [*Scanlon et al.*, 2007] and the influence of the topography of the upper boundary [*Cardenas*, 2007; *Haggerty et al.*, 2002; *Kirchner et al.*, 2001; *Worman et al.*, 2007]. All of these processes are shown to be scale dependent, for example the influence of a topographical upper boundary to groundwater flow may range in scale from streambed ripples to the land surface up to the continental scale. The work presented here, uses a fully-integrated, numerical watershed model that incorporates aspects of all these systems demonstrates scale dependence and points to the relative importance of these various component processes.

For the case of steady state conditions and based on the assumption that the water table closely follows the topography of the upper boundary, one can show that topography induces groundwater flow with power law or fractal behavior even if the subsurface is homogeneous. This stems from the presence of stagnation points in the domain, i.e. locations where the flow velocities are zero. These stagnation points generate velocity distributions over a wide range of scales that lead to a wide range in residence time distributions of groundwater [*Cardenas*, 2007]. In addition, subsurface heterogeneity can enhance power lower behavior of residence time distributions by additionally producing a range of groundwater velocities and thus residence time distributions [*Haggerty et al.*, 2000]. The self-similarity of groundwater systems has also been observed by many authors (e.g. [*Worman et al.*, 2007]). In a purely hydraulic sense, this self-similarity is evident from an examination of the classical Toth solution [*Toth*, 1963]. Expressed in non-dimensional variables, the solution is valid on all spatial scales as long as Darcy flow is guaranteed. Therefore, one can “zoom” in and out of the potential solution from the streambed scale to the continental scale without changing the basic mechanisms, which is one of the central requirements of self-similarity.

The aforementioned studies are based on a suite of assumptions such has steady state conditions of the potential field and that processes of the vadose zone and at the land surface do not exert any influence on subsurface flow, i.e. only flow in the saturated zone is considered. However, even if there is a free water table that closely follows the topography, it may be dynamic due to diurnal and seasonal variations in atmospheric forcing and vegetation. In this case, a steady state solution of the potential field does not suffice. Thus, in order to examine the influence of the land surface and the shallow subsurface on the residence time distributions of groundwater, one requires a more advanced analysis that takes into account the pertinent physical processes, such as three-dimensional variably saturated groundwater flow, root water uptake by plants, evaporation, from the bare soil, infiltration, and overland flow. This has been discussed previously by *Reed et al.*, [2006], who pointed to the need for field measurements on the watershed scale and the development of simulation tools treating the subsurface-land surface-atmosphere system in an integrated fashion.

In this study, a novel watershed simulation platform is applied to a catchment with an area on the order of $10^3 km^2$. The simulation platform consists of a parallel, three-dimensional, variably saturated groundwater/surface water flow code, coupled to a land surface model. This fully-coupled model accounts for pertinent processes at, across and below the land surface and is forced by an atmospheric time series, thus, relaxing many of the assumption made in previous studies. Transient particle tracking of a conservative tracer is used to derive residence time distributions of parcels of water recharged either at the water table or at the land surface (thus being influenced by vadose and root zone processes) for a range of macrodispersion. In the ensuing analysis, the power spectra of the distributions of residence time and their slope are computed. The different slopes of the power spectra are related to the simulated processes and to the statistical concept of stationarity.

Methods

In order to arrive at residence time distributions that were used in the spectral analysis, a two-step numerical experiment was performed. First, an integrated watershed simulation platform was applied to a watershed in central Oklahoma (USA), which resulted in a time series of three-dimensional pressure fields in the subsurface. Second, a Lagrangian, particle-tracking method was applied in conjunction with these transient pressure results to develop residence time distributions of subsurface water for the ensuing spectral analysis. Both steps are outlined in more detail below.

Integrated Watershed Simulations

The pressure fields for the particle tracking experiment were obtained from simulations using an integrated watershed numerical code. The methodology and simulation are described in detail in *Kollet and Maxwell* [2007]. The numerical code consists of ParFlow, a parallel, three-dimensional variably saturated groundwater/surface water flow code with an integrated land surface model. The land surface model is the Common Land Model (CLM, [*Dai et al.*, 2003]) and calculates the mass and energy balance at the land surface. ParFlow calculates the moisture redistribution in the shallow subsurface that is influenced by evapotranspiration and infiltration as well as deep groundwater flow. For technical details we refer the reader to [*Ashby and Falgout*, 1996; *Jones and Woodward*, 2001; *Kollet and Maxwell*, 2006; *Kollet and Maxwell*, 2007; *Maxwell and Miller*, 2005].

As described in detail in *Kollet and Maxwell* [2007] the simulation platform was applied to the Little Washita watershed, Oklahoma, USA for the water-year 1999. This model of the Little Washita watershed consisted of a deep, homogeneous aquifer (~10^2m), topography, spatially distributed land and soil cover, and overland flow parameters. A one year time series of spatially uniform atmospheric forcing was applied from September 1998 until August 1999 in spinup mode until a dynamic equilibrium was obtained. The spinup procedure resulted in the development of the Little Washita River in the model domain that is the locus of particle injection in the particle tracking experiment.

Residence Time distributions and Spectral Analysis

A Lagrangian, particle-tracking approach, described in detail in previous work [*Maxwell and Kastenberg*, 1999; *Maxwell et al.*, 2003; *Maxwell and Tompson*, 2006; *Maxwell et al.*, 2007; *Tompson et al.*, 1998], was used to simulate the evolution of age of tagged parcels of water. Particle-tracking methods have been widely applied in subsurface transport problems [e.g., *LaBolle et al.*, 1996; *Tompson and Gelhar*, 1990]. This particular particle model has been previously applied to simulate water age and to interpret isotopic observations [e.g., *Maxwell et al.*, 2003; *Tompson et al.*, 1999]. Lagragian methods are advantageous in that they allow for rapid simulation of transport and do not suffer from numerical dispersion, making them well-suited for representing accurately transport with very large Peclet numbers.

For this simulation, particles placed at the bottom of fully saturated riverbed cells, located within the primary watershed, at a density of 5,000 particles per grid cell for a total number of particles, Np=765,000. Pressure fields advanced daily for 500 years for a total of 182,500 timesteps, i.e. the pressure field time series from the one year spinup was averaged daily and repeated 500 times. As in *Tompson et al.,* [1999] and *Maxwell et al.*, [2003], cell velocities are reversed and particles are transported backwards to the source location. All pressure fields are taken from the results of *Kollet and Maxwell* [2007] as mentioned above. For the water table cases (case WT), to mimic an isotopic tracer such as ^{3}H that will re-equilibrate when exposed to the atmosphere, particles were stopped when the saturation dropped below 0.95 and their travel time were recorded. For the vadose zone cases (case LS) particles were not stopped until they reached the land surface. Macrodispersion was added to these transport simulations to represent the dispersive effect of subsurface heterogeneity on transport. While a very approximate representation, this approach allowed for varying the Peclet number,*Pe*, ($\sim L/\alpha_l$) by varying the longitudinal dispersivity over four orders of magnitude and using a hillslope scale of L = 7.5km from *Kollet and Maxwell* [2007] (Table

1). For all simulations the transverse dispersivity was set to $\alpha_l/10$. An example of the spatial distribution of travel time generated using this approach may be seen in Figure 1.

The time distributions created by these reverse particle traces were then binned into one-day increments to create a probability distribution function (PDF) of travel times from any recharge point to the riverbed. Due to the discrete nature of particle tracking, some of the PDF bins contained zero values which were omitted creating an unevenly sampled distribution. These PDF's where then transformed into the spectral domain using the so-called Lomb-Scargle technique for uneven data [*Lomb*, 1976; *Scargle*, 1982] as implemented by *Press et al.,* [1996]. The resultant spectral power-wavelength plots are shown in Figures 2 and 3.

Table 1. Parameter summary for the 8 simulated transport cases.

Case	*Pe*	α_l (m)
WT	75000	0.1
	7500	1
	750	10
	75	100
LS	75000	0.1
	7500	1
	750	10
	75	100

Results and Discussion

Figures 2 and 3 show the power spectra of the residence time distributions calculated from particle path simulations ending at the water table, case WT, and at the land surface, case LS. In all simulations the spectra exhibit power law behavior and fractal scaling that has been observed previously in experimental and theoretical studies [e.g., *Kirchner et al.*, 2000]. Increases in macrodispersion (i.e. a decrease in *Pe* due to an increase in longitudinal dispersivity) act as a low-pass filter and smooth the curves similar to the moving average that is also shown in Figures 2 and 3. Since, the analysis is based on a pressure distribution time series repeating one year of spinup 500 times resulting in a total simulation time of 500 years, the correlation length of the residence time distribution appears to be one year.

In case WT (Figure 2), the slopes of the power spectra, *m*, first increase with increasing heterogeneity and then decrease and range between $0.87<m>1.16$. This dependence of *m* on *Pe* is also illustrated in Figure 4. The range *m* corresponds well with reported values in the literature from experimental and theoretical studies. For example, *Kirchner et al.*, [2000] obtained similar values from the analysis of chloride concentrations from small catchments (~$10^0 km^2$) at the Welsh coast line and nine other catchments spanning a variety of climate and hydrologic conditions. In theoretical studies, *Kirchner et al.*, [2001] only obtained model results that produced fractal scaling by using very large macrodispersivities, i.e. $Pe \leq 1$. Thus, the range of *m* obtained from the measured data was explained by the degree of heterogeneity. The results presented here in Figure 2, however, show fractal scaling for *Pe* values up to 75,000, many orders of magnitude larger than previous studies. This is a confirmation of previous results that an undulating topography, which is directly accounted for in the current work, plays a significant role in the apparent macrodispersion of residence times of parcels of water in the subsurface [e.g., *Worman et al.*, 2007]. This study demonstrates that the influence of topography persists also under transient conditions.

In previous scaling analysis, vadose zone or root zone processes have not been considered. Some tracers such as chloride, used in the work of *Kirchner et al.*, [2000], as opposed to isotopic tracers, do not re-equilibrate when exposed to the atmosphere. Chloride residence times will then reflect the time history of pathways between the ground surface and water table. Thus, vadose zone processes, previously ignored by other studies, need to be considered in the analysis. Figure 3 shows the power spectra for case LS, where the vadose and root zone are included in the simulations of travel times. Inspection of the spectra for different *Pe* values shows that *m* of the power spectra increases more continuously with increasing heterogeneity than for the case WT. This is also shown in Figure 4. The slopes now range between $1.04<m>1.38$. In case of *Pe*=75, the power law behavior appears to weaken for larger time scales and approaches a more exponential behavior.

Juxtaposition of Figure 2 and 3 show directly the influence of the vadose zone on the residence time distribution spectra for varying degrees of macrodispersion. This is summarized in Figure 4. The vadose zone generally increases the slope of the power spectra, and thus introduces longer range correlations, which can be explained by differences in the variances in the residence time distributions. Processes in the vadose zone also introduce more noise in the power spectra (as shown in Figure 3). This might be because particles become "locked" in the vadose zone through continuous redistribution due to evapotranspiration and infiltration. Vadose and root zone processes may, in a sense, introduce additional stagnation points, similar to those found in the classical Toth problem analysis, and introduction of macrodispersion may smooth the effects of those stagnation points on the power spectra of the age distribution. These stagnation points appear to be important in explaining the scaling behavior of a watershed, however, as large dispersivities appear to destroy this structure to an extent not observed in physical systems.

It has been shown previously, that the slope of the power spectra is a measure of stationarity of the data [*Davis et al.*, 1994], where stationarity means that the statistics of the data do not depend on translation along the independent coordinate. For stationary cases, *m* is generally smaller than one and for nonstationary cases, *m* is generally larger than 1. Thus, in the simulations presented here, for *Pe*>7500 and in absence of a vadose zone, macrodispersion appears to increase stationarity and the residence time distributions approach white noise to '1/*f*' noise [*Davis et al.*, 1994]. On the other hand, in case LS, the macrodispersion in conjunction with processes of the vadose zone have the opposite effect. The slope of the power spectrum is larger than one and increases with increasing macrodispersion, which suggests nonstationarity. Thus, the vadose zone being a relatively thin interface has a significant influence on residence time distributions, because of the non-linearity of variably saturated flow and evapotranspiration, which depends on the moisture state of the shallow subsurface.

Summary

Using a fully-coupled, groundwater, vadose zone and land surface model in conjunction with a Lagrangian particle tracking model a series of residence time distributions were developed for recharge from the land surface and water table to the riverbed. A spectral analysis of these residence times demonstrated power spectra that exhibit power-law or fractal type behavior previously observed in experimental studies for a wide range of *Pe* numbers. In age distribution cases where the effects of vadose zone processes were not considered, increasing macrodispersion first increases, then decreases the slope of the log-log power spectra below one. In contrast, consideration of vadose and root zone processes on residence time distributions leads to increasing slopes of the log-log power spectra with increasing macrodispersion and slopes always greater than one. Thus, the vadose zone interface of the shallow subsurface has a profound influence on the scaling behavior of the residence time distribution. Following the notion of the slope of the power spectra, *m,* being a measure of stationarity, the vadose zone decreases stationarity of the residence time distribution. That fractal scaling is demonstrated for much larger *Pe* numbers than in previous studies confirms the importance of topographic also under transient conditions. However, the presented study also shows the influence of land surface and vadose zone processes on the apparent macrodispersion of solutes in groundwater. This indicates that the observed fractal scaling behavior in watersheds might be explained through a combination of these physical processes.

The presented study provides a picture of overall fractal scaling of solutes in watersheds in an integrated fashion i.e. combining various aspects such as topography, macrodispersion, the vadose zone, and land surface processes that have been discussed separately in the literature. The results also suggest that the simulation platform is useful in analyzing path and residence time distributions in real-world system by appropriately capturing the variances over a large range of scales.

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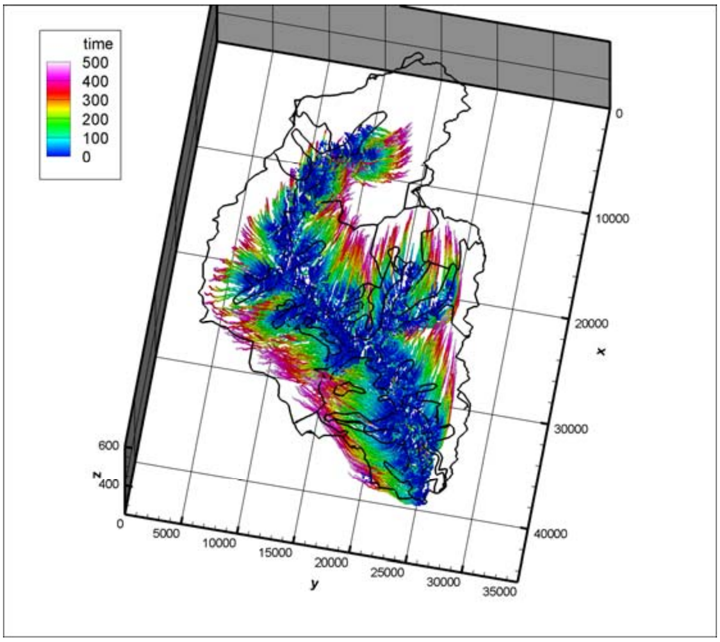
Figure Captions

Figure 1. Three dimensional plot of backwards in time streamlines for the Little Washita watershed. Particle ages are depicted along each pathline in years. The watershed outline is plotted as the solid black line. The time scale is in years of traveltime.

Figure 2. Logarithmic plot of spectral power as a function of wavelength for different values of dispersivity (noted by the Peclet number in each figure) for simulations ending at the water table (case WT). Note that raw spectra are shown in gray, smoothed spectra in black and a linear fit of the spectra shown with the dashed line with the slope (m) given for each case.

Figure 3. Logarithmic plot of spectral power as a function of wavelength for four different values of dispersivity (noted by the Peclet number in each figure) for simulations ending at the ground surface, thus, including vadose zone processes (case LS). Note that raw spectra are shown in gray, smoothed spectra in black and a linear fit of the spectra shown with the dashed line with the slope (m) given for each case.

Figure 4. Semi-logarithmic plot of the slope (m) of a best linear fit to the power spectra as a function of Peclet number for vadose (case LS, triangles) and non-vadose zone (case WT, squares) cases.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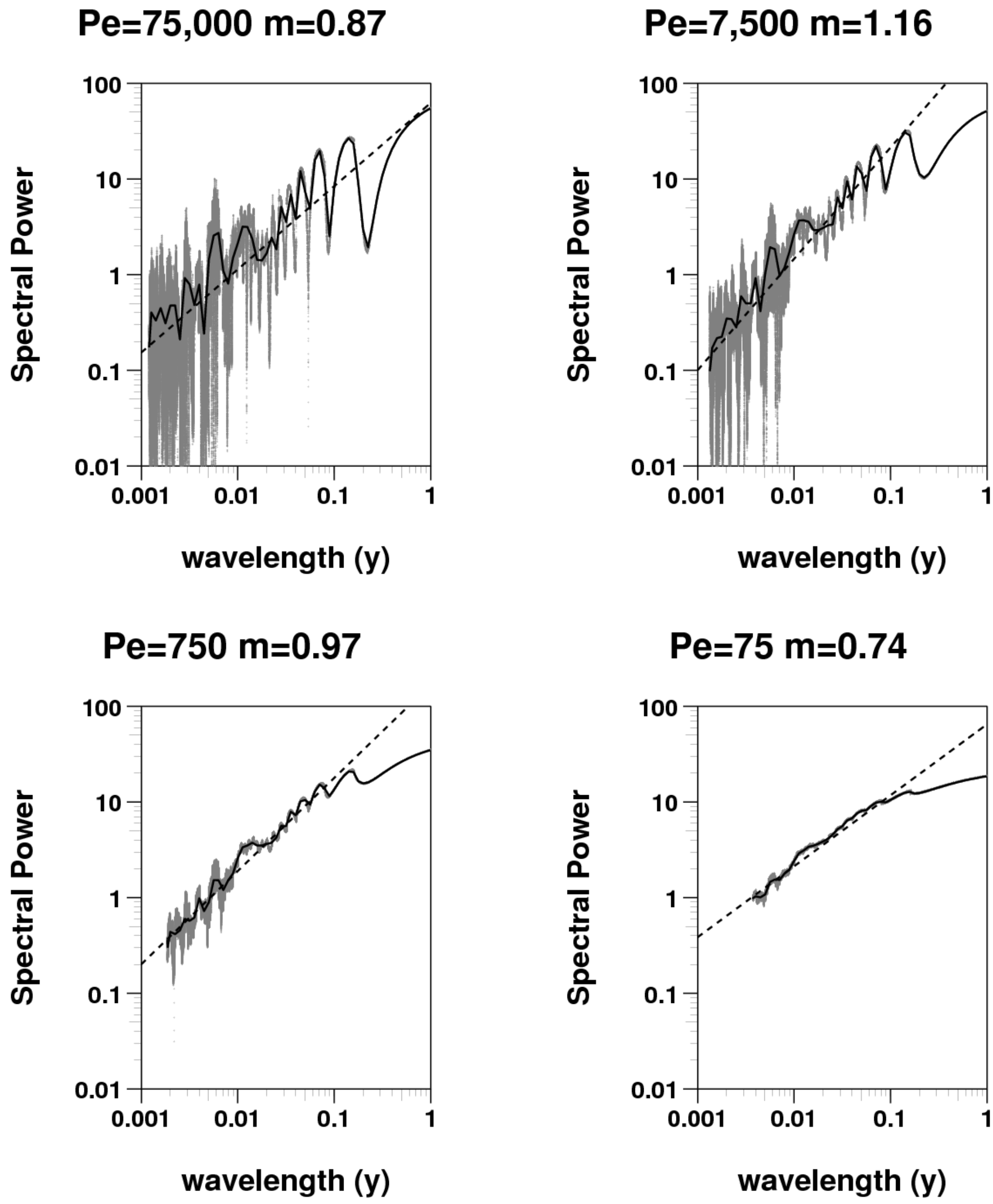
y

Figure 1.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Pe=7,500 m=1.16
Pe=750 m=0.97
Pe=75 m=0.74
Spectral Power
wavelength (y)
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10
1
0.1
0.01
0.001
0.01
0.1
1

Figure 2.

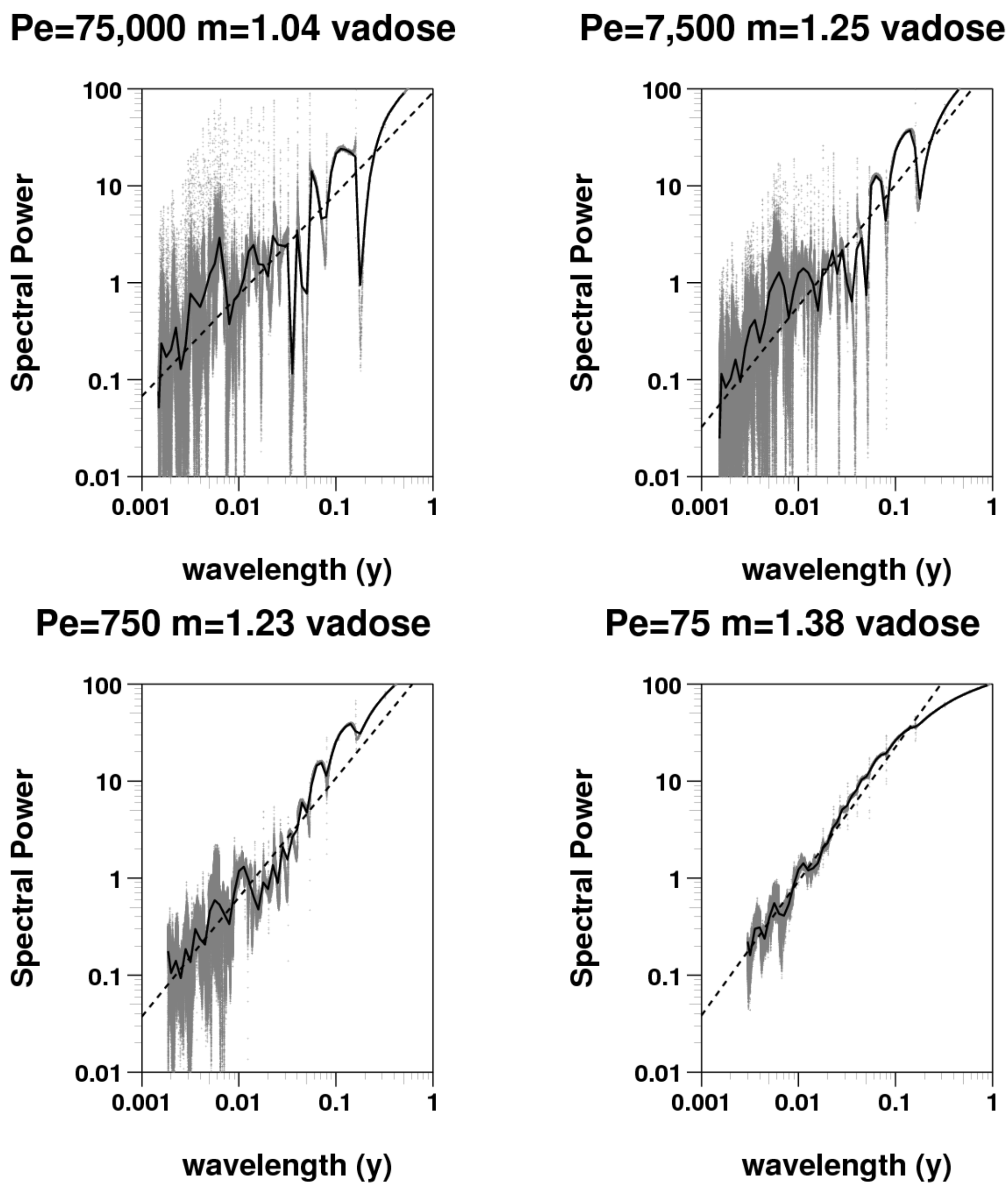
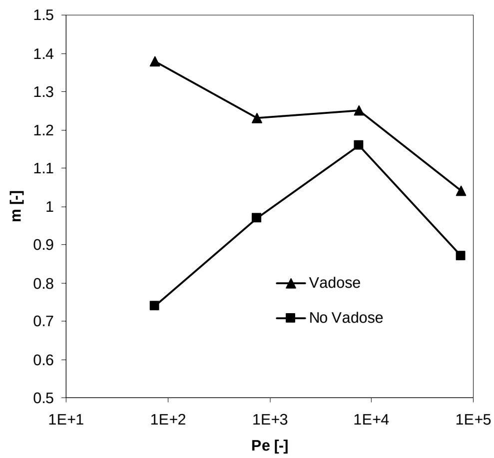

Pe=75,000 m=1.04 vadose
Pe=7,500 m=1.25 vadose
Pe=750 m=1.23 vadose
Pe=75 m=1.38 vadose
Spectral Power
wavelength (y)
100
10
1
0.1
0.01
0.001
0.01
0.1
1

Figure 3.


1.5
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m [-]
Vadose
No Vadose
1E+1
1E+2
1E+3
1E+4
1E+5
Pe [-]

Figure 4.